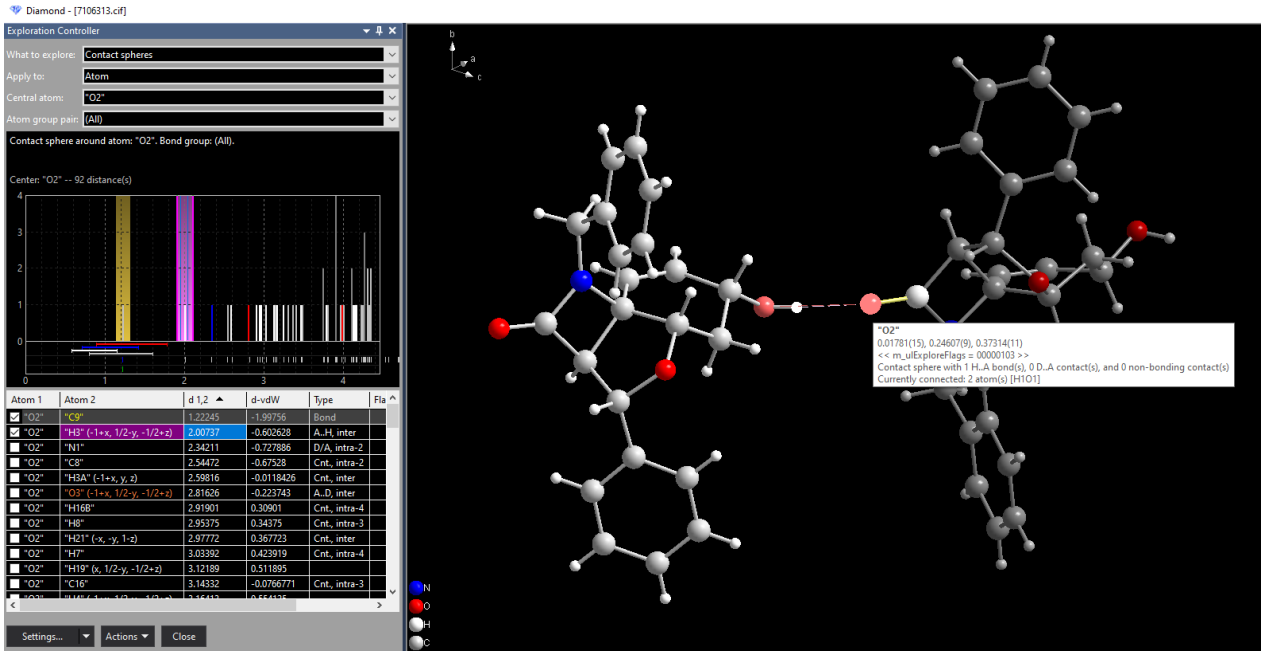
DIAMOND

Crystal and Molecular Structure Visualization



New Version 5

The new Diamond version 5 contains several new features:

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The most outstanding new feature is the **Exploration View,** which enables to study (strong) bonds as well as H-bonds and non-bonding contacts when checking for neighbouring atoms and molecules. A bond (or contact or H-bond, rsp.) can be added or removed by clicking the checkmark in the distance table or shifting the boundary in the histogram or by clicking on the bond/contact in the structure picture graphics (see screenshot above).

The commands *Take Picture* and *Continue With New Picture* offer an improved workflow when creating multiple pictures for a structure data set.

The *More Pictures* docking window and the *Caption Bar* give a simplified overview of structure pictures.

Settings can be imported from version 4.

A newer version of Crystallography Open Database (COD; www.crystallography.net) is available.

More outstanding functions:

- ✓ Import with automatic format recognition
- ✓ Build up structure pictures automatically or manually
- ✓ Schemes (style sheets) for building and design
- ✓ Structure type database
- ✓ Ellipsoids, disorder, mixed sites
- ✓ Molecules, packing diagrams
- ✓ Polymers and molecule clusters
- ✓ Fragmentated and broken-off bonds
- ✓ H-bonds and non-bonding contacts
- ✓ Preview of neighbouring atoms and -molecules
- ✓ Atomic environments from Dirichlet domains
- ✓ Coordination and Voronoi polyhedra
- ✓ Atom vectors, labels, and free text
- ✓ Reflection parameters and diffracion diagrams
- ✓ Distances, angles, and torsion angles
- ✓ hkl- and L.S.-planes and lines
- ✓ 3D export to POV-Ray, OBJ, and STL
- ✓ Video sequences and animations

Diamond version 5 will be/has been released in October 2023. The **update from Diamond 4 to 5** is **free-of-charge**.

https://www.crystalimpact.de/diamond/Default.htm

Price* for new License	*academic*	*regular*
Semiannual license (6 months)	149,50 €	299 €
Annual license (12 months)	299 €	598 €
Single license (permanent)	599 €	1.198 €
Site license (permanent)	1.198 €	2.396 €
Campus license (permanent)	2.396 €	4.792 €

* Prices do not include taxes which may be due.

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